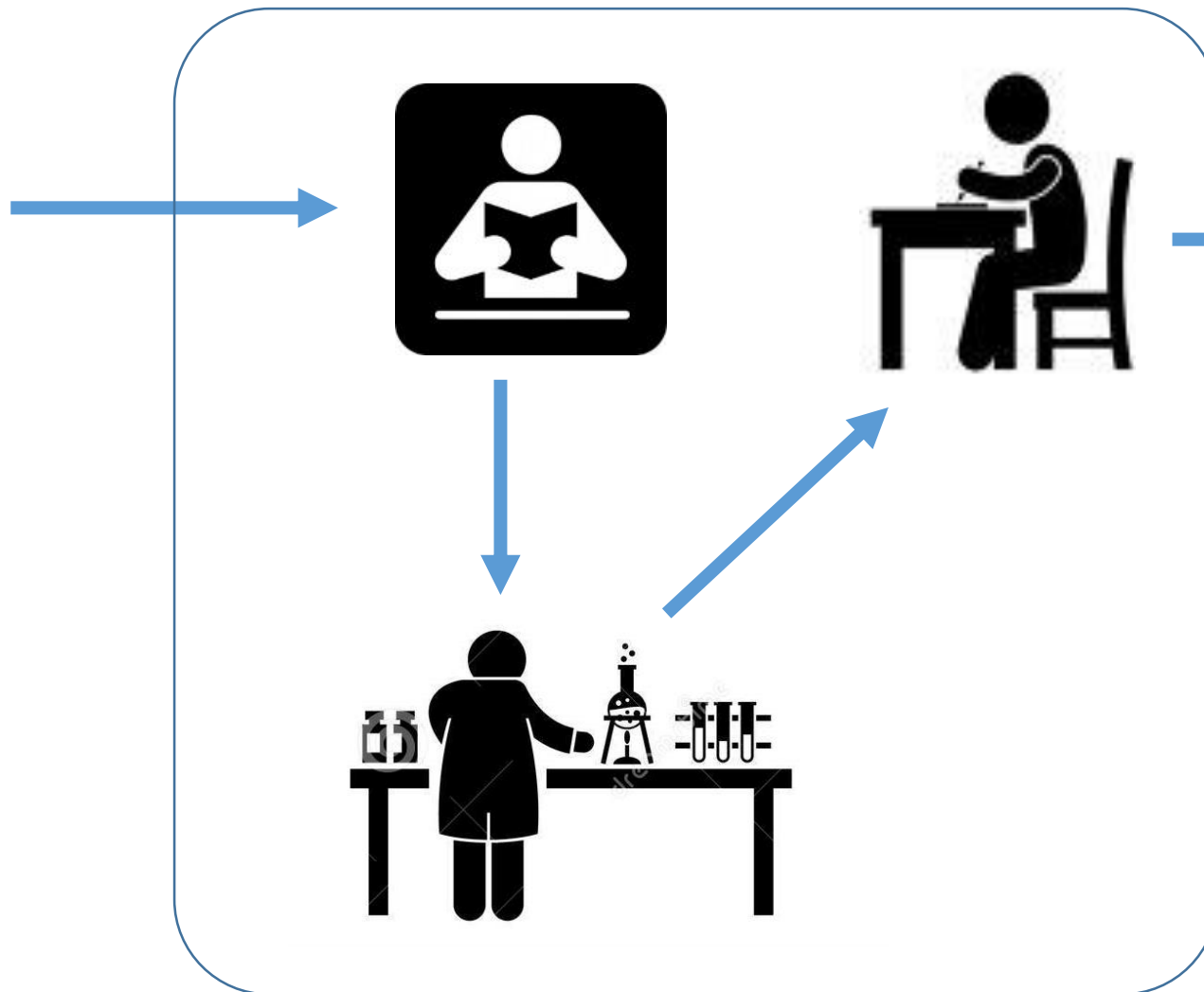


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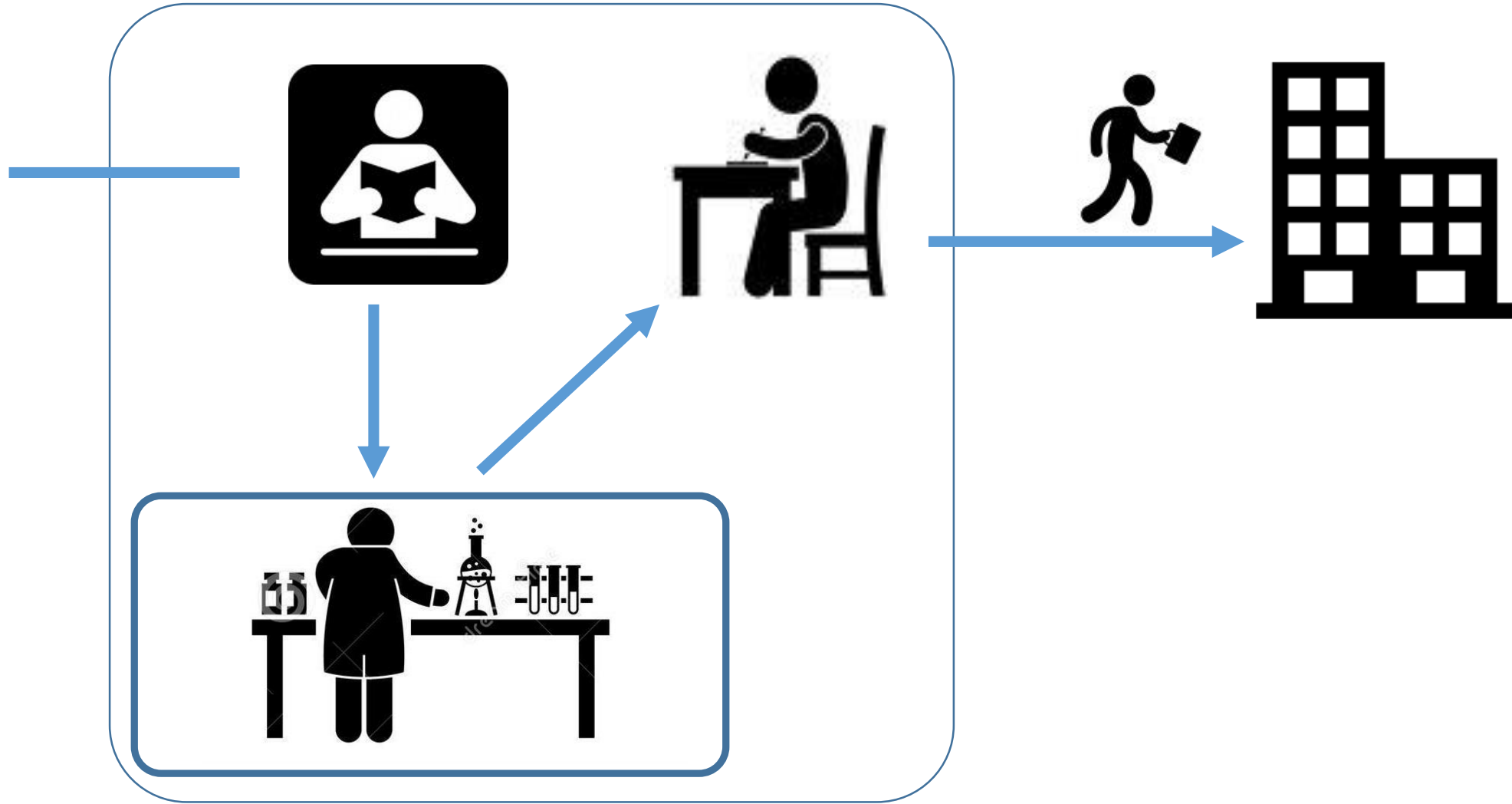
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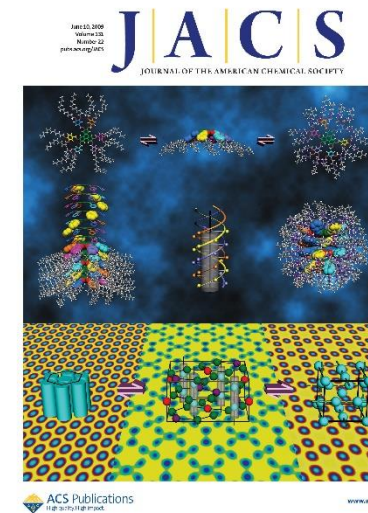
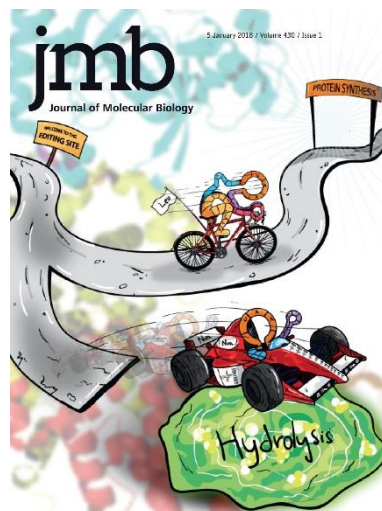
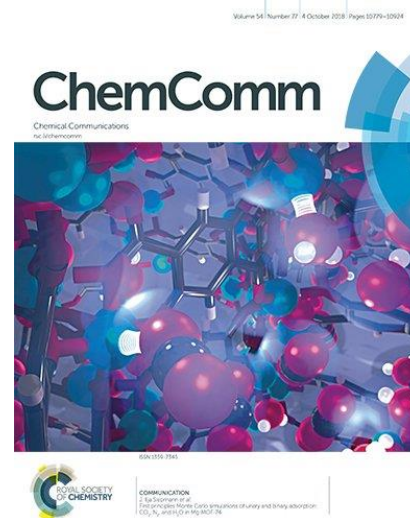
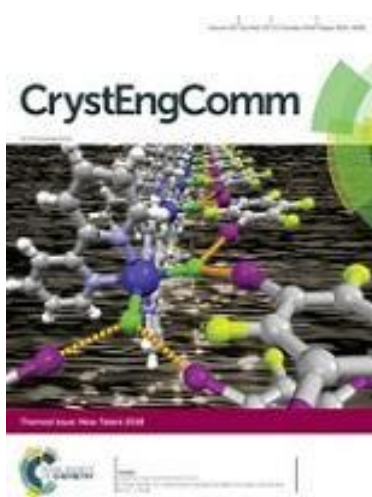
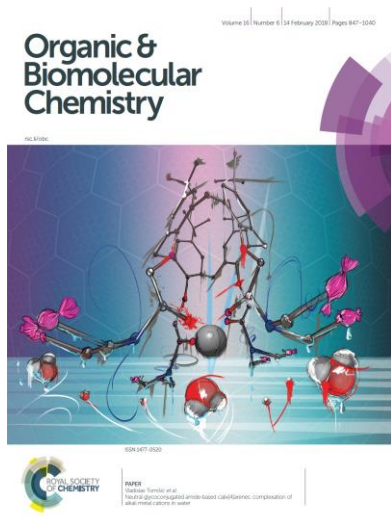


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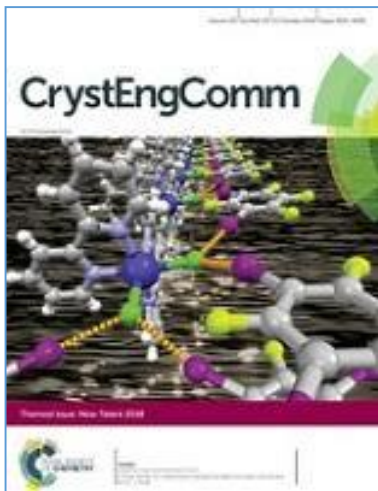


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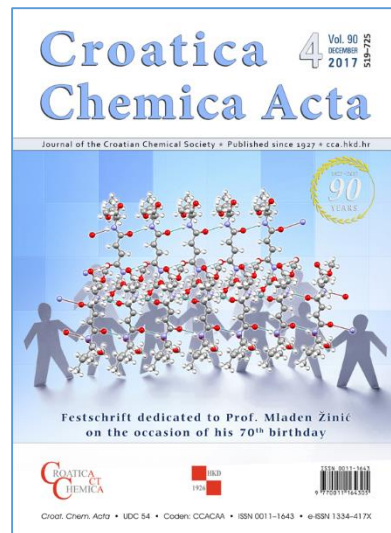
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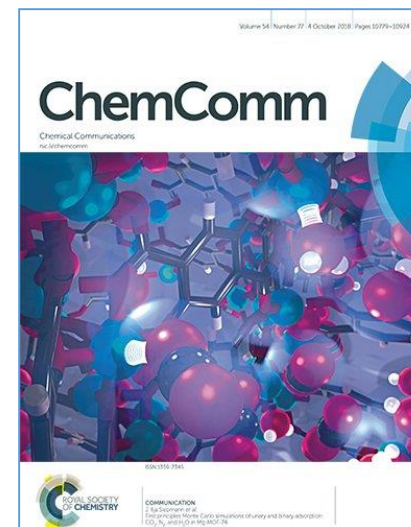


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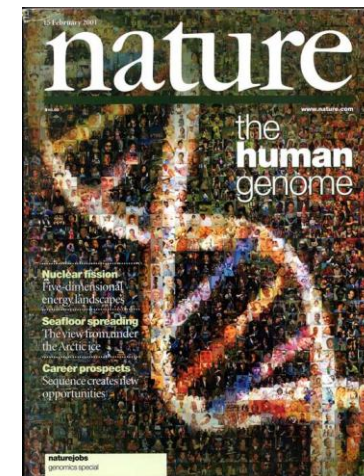


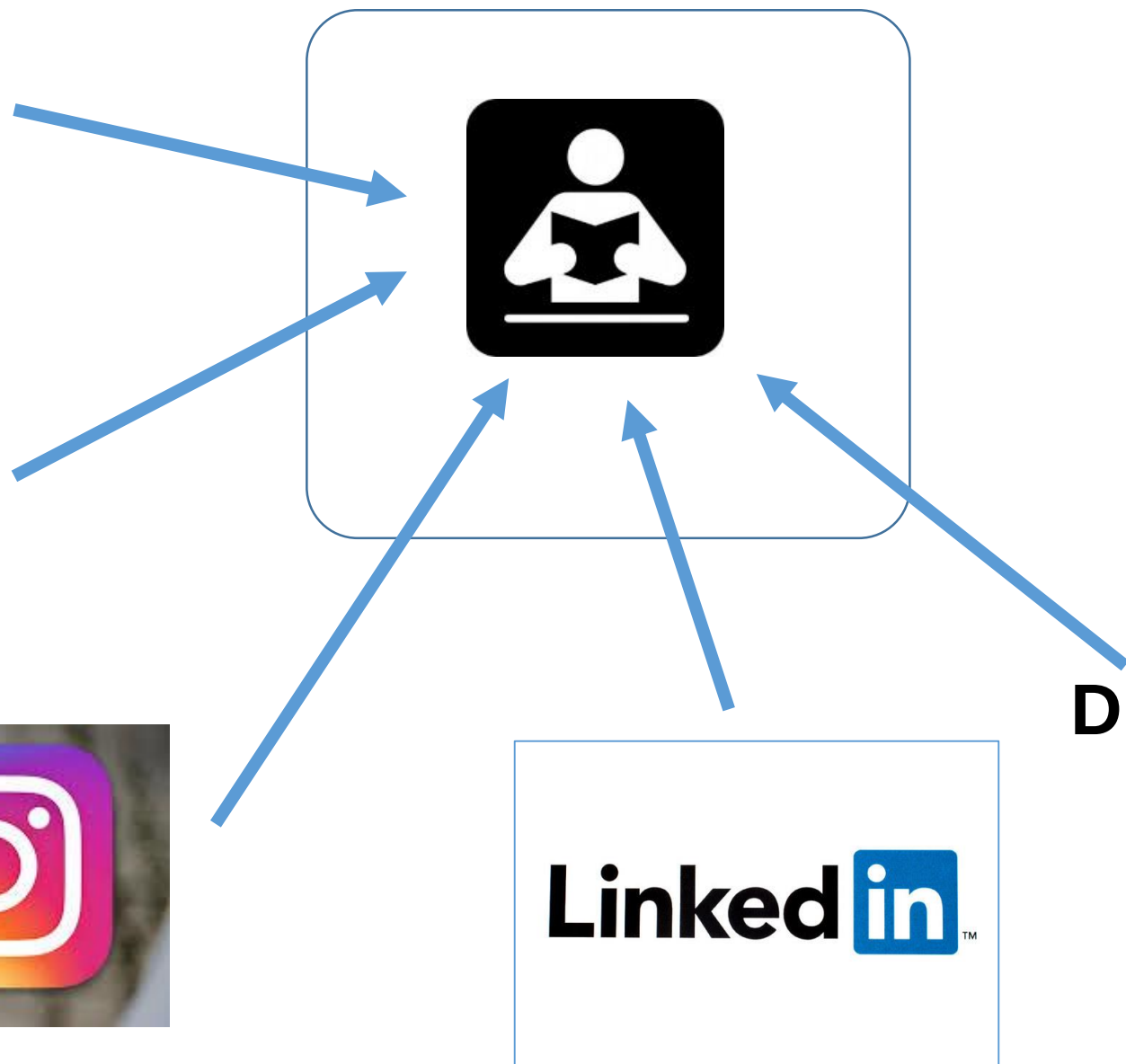
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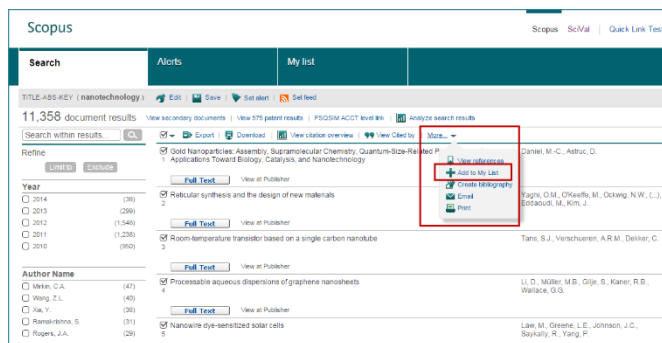
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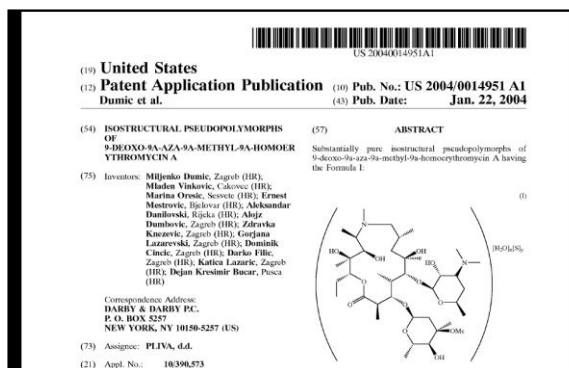


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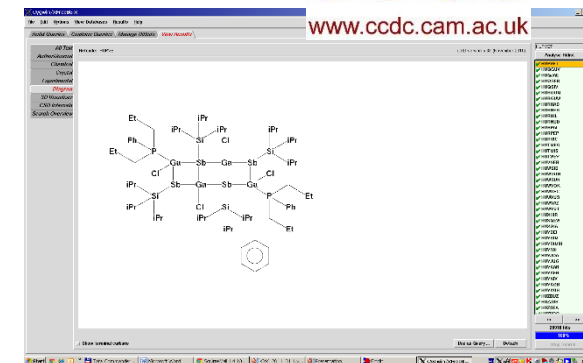
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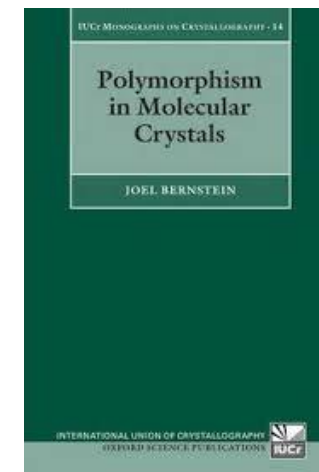
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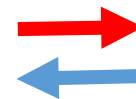
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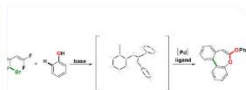
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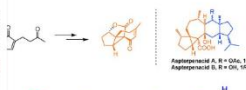
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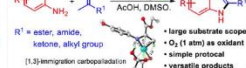
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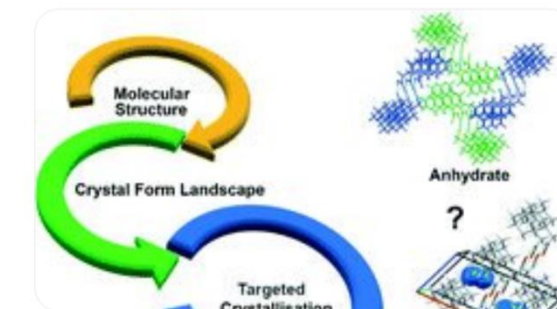
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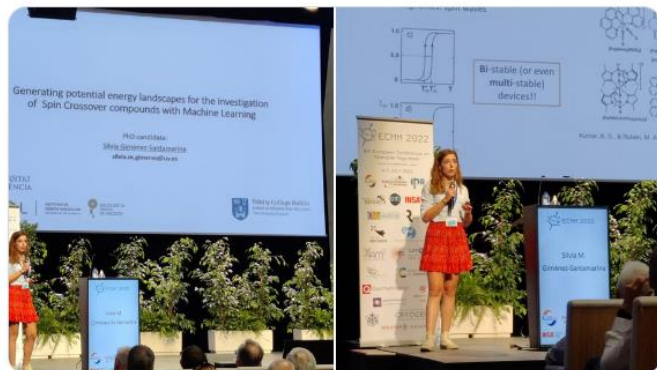
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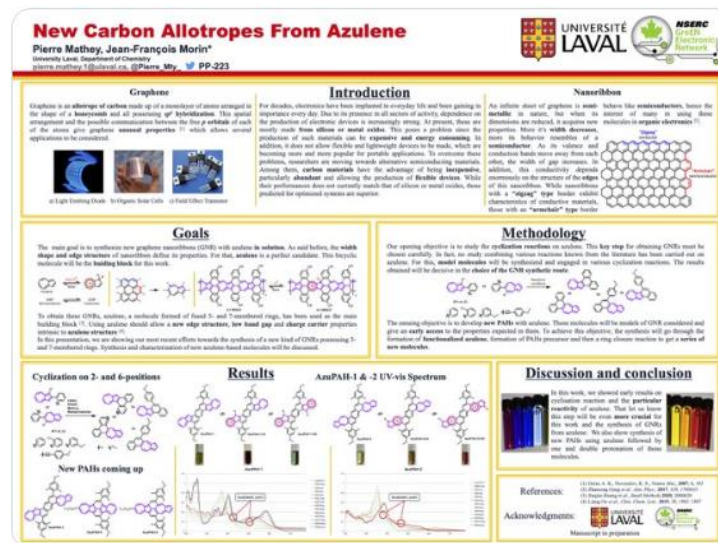
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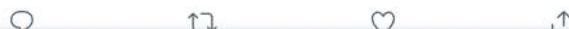
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Halogen-bonded cocrystals of *N*-salicylidene Schiff bases and iodoperfluorinated benzenes: hydroxyl oxygen as a halogen bond acceptor



[Andrea Carletta](#)^a [Marija Zbaňnik](#)^b [Matea Vitković](#)^b [Nikolay Tumanov](#)^b [Vladimir Stilić](#)^{a,b} [Johan Wouters](#)^{a*} and [Dominik Cincić](#)^{a,b}

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Abstract

To explore the halogen bonding proclivity of the *o*-hydroxyimine hydroxyl group, we have prepared two imines as halogen bond acceptors: salicylideneaniline (I) and a 3-pyridyl analogue (II) derived from the condensation of salicylaldehyde and 3-aminopyridine. These two Schiff bases were selected as the two simplest representatives of *o*-hydroxyimines, where one (II) possesses a potentially competing halogen bond acceptor (pyridine nitrogen) and the other does not. For cocrystal screening, as halogen bond donors, we used perfluorinated iodobenzenes: 1,2-, 1,3-, 1,4-diiodotetrafluoro-benzene (**12tfib**, **13tfib**, and **14tfib**) and 1,3,5-triiodotrifluoro-benzene (**135tfib**). The hydroxyl group has been found to act as a halogen bond acceptor in three out of five crystal structures determined in this study: (II)(**13tfib**), (II)(**135tfib**) and (II)₂(**135tfib**). In all three cases, a pyridine nitrogen is also employed in halogen bonding. Our attempts at preparing cocrystals of I were generally unsuccessful and the only cocrystal of I, which has been obtained, with **14tfib**, does not exhibit a halogen bond involving a hydroxyl oxygen. These results suggest that the halogen bond motif with an isolated hydroxyl group as the acceptor seems to be less favourable than the previously studied bifurcated halogen bonding motif with the *ortho*-methoxy hydroxyl group as the acceptor.

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The crystal structure determination of sodium chloride in 1913,¹ which was a consequence of Max von Laue's diffraction of X-rays from single crystals of copper sulfate² as well as of the postulation of Bragg's law³ the previous year, marks the beginning of a new era in solid-state chemistry and the science of crystallography.⁴ During the century following these

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